

=> file reg
FILE 'REGISTRY' ENTERED AT 15:21:03 ON 26 APR 2002
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STRUCTURE FILE UPDATES: 25 APR 2002 HIGHEST RN 408304-53-0
DICTIONARY FILE UPDATES: 25 APR 2002 HIGHEST RN 408304-53-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
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Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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(FILE 'HOME' ENTERED AT 14:27:54 ON 26 APR 2002)

FILE 'LREGISTRY' ENTERED AT 14:29:14 ON 26 APR 2002
L1 STR

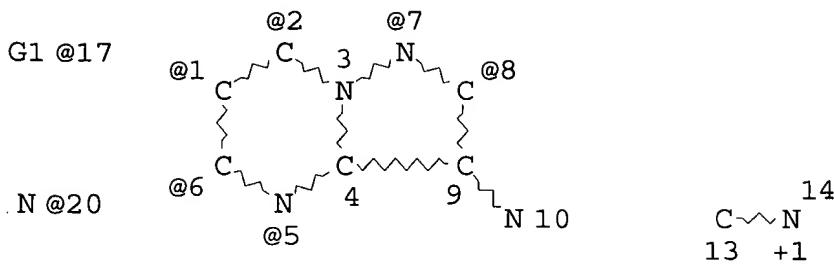
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L2 3 S L1
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L5 STR L3
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L7 27 S L5 FUL
SAV L7 KOS503/A

FILE 'CAOLD' ENTERED AT 15:11:08 ON 26 APR 2002
L8 0 S L7

FILE 'ZCAPLUS' ENTERED AT 15:11:08 ON 26 APR 2002
L9 1 S L7

FILE 'REGISTRY' ENTERED AT 15:21:03 ON 26 APR 2002

=> d 17 que stat
L5 STR



VAR G1=OH/20
VPA 17-8/7/2/1/6/5 U

NODE ATTRIBUTES:

CHARGE IS E+1 AT 14
NSPEC IS RC AT 13
NSPEC IS RC AT 14
NSPEC IS RC AT 20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L7 27 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 4282 ITERATIONS
SEARCH TIME: 00.00.02

27 ANSWERS

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 15:21:18 ON 26 APR 2002
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FILE COVERS 1907 - 26 Apr 2002 VOL 136 ISS 17
FILE LAST UPDATED: 24 Apr 2002 (20020424/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d 19 1 ibib_abs-hitstr hitrn

L9 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:513700 ZCPLUS
 DOCUMENT NUMBER: 133:136754
 TITLE: Novel cationic oxidation bases with a pyrazolo[1,5-a]pyrimidine structure, their use for oxidation dyeing of keratin fibers, dyeing compositions et dyeing methods
 INVENTOR(S): Terranova, Eric; Fadli, Aziz; Lagrange, Alain
 PATENT ASSIGNEE(S): L'oreal, Fr.
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000043396	A1	20000727	WO 2000-FR73	20000114
W: AE, AL, AM, AT, AU, AZ, BA, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2788522	A1	20000721	FR 1999-503	19990119
FR 2788522	B1	20010216		
EP 1147109	A1	20011024	EP 2000-900581	20000114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.:			FR 1999-503	A 19990119
			WO 2000-FR73	W 20000114

OTHER SOURCE(S): MARPAT 133:136754
 AB The invention concerns novel 4-aminopyrazolo[1,5-a]pyrimidines comprising a cationic group Z, Z being selected among quaternized aliph. chains, aliph. chains comprising a quaternized ring, and their use as oxidn. base for dyeing keratin fibers, the dyeing compns. contg. them, and the oxidn. dyeing

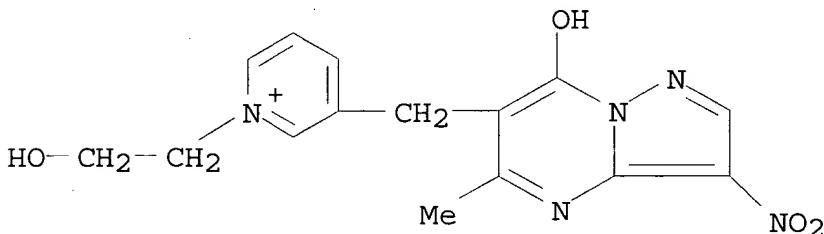
methods using them. These compds. allow dyeing of keratin fibers so that individual strands have multiple shades. Thus, reaction of 50 g 4-nitro-1H-pyrazol-3-ylamine hydrochloride 12 h at reflux with 60 g Et acetoacetate in HOAc, chlorination of 23.3 1st intermediate 2.5 h at reflux with 230 cm³ POCl₃ in presence of 15.4 g PhNMe₂, reaction of 4.5 g 2nd intermediate 2 h with 2.88 g 3-imidazol-1-ylpropylamine in a DMF-dioxane mixt. in presence of Et₃N, reaction of 3 g 3rd intermediate 6 h at reflux with 10 g 2-chloroethanol, and redn. of the 4th intermediate gave 3-[3-(3-amino-5-methylpyrazolo[1,5]pyrimidin-7-ylamino)propyl]-1-(2-hydroxyethyl)-3H-imidazol-1-ium chloride, which was isolated as the dihydrochloride.

IT 286373-91-9P

(quaternary ammonium base precursor; quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)

RN 286373-91-9 ZCAPLUS

CN Pyridinium, 1-(2-hydroxyethyl)-3-[(7-hydroxy-5-methyl-3-nitropyrazolo[1,5-a]pyrimidin-6-yl)methyl] -, chloride (9CI) (CA INDEX NAME)

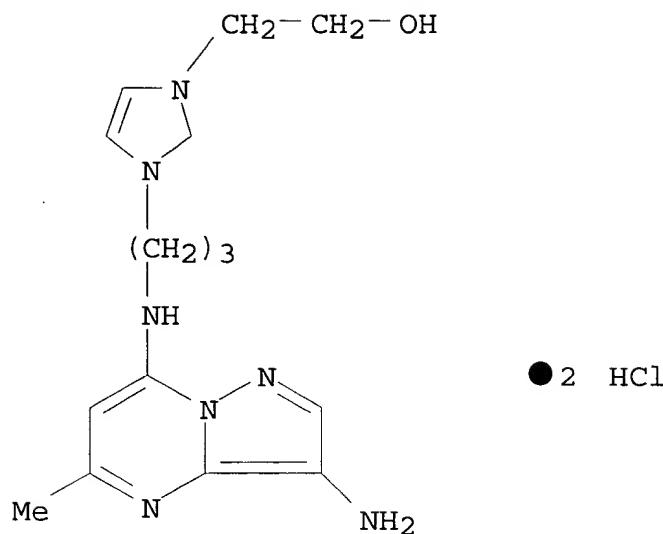
● Cl⁻

IT 286373-84-0P 286373-87-3P 286373-92-0P
 286373-94-2P 286373-96-4P 286373-98-6P
 286374-00-3P 286374-02-5P 286374-04-7P
 286374-05-8P 286374-07-0P 286374-08-1P
 286374-10-5P 286374-11-6P 286374-13-8P
 286374-14-9P

(quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)

RN 286373-84-0 ZCAPLUS

CN 1H-Imidazolium, 1-[3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-3-(2-hydroxyethyl) -, chloride, dihydrochloride (9CI) (CA INDEX NAME)

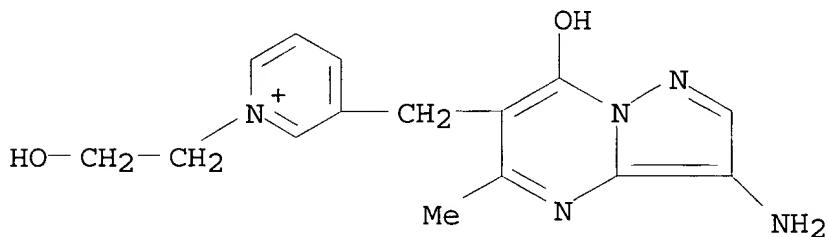


● Cl⁻

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

RN 286373-87-3 ZCPLUS

CN Pyridinium, 3-[(3-amino-7-hydroxy-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)methyl]-1-(2-hydroxyethyl)-, chloride, monohydrochloride (9CI)
(CA INDEX NAME)



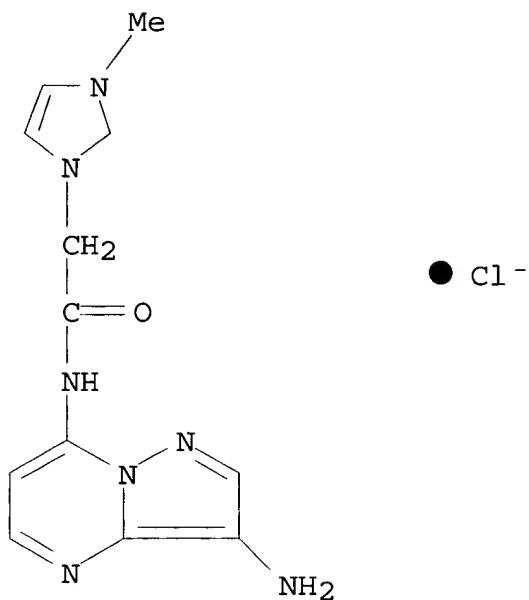
● Cl⁻

HCl

RN 286373-92-0 ZCPLUS

CN 1H-Imidazolium, 1-[(2-[(3-aminopyrazolo[1,5-a]pyrimidin-7-yl)amino]-2-

oxoethyl]-3-methyl-, chloride (9CI) (CA INDEX NAME)



*** FRAGMENT DIAGRAM IS INCOMPLETE ***

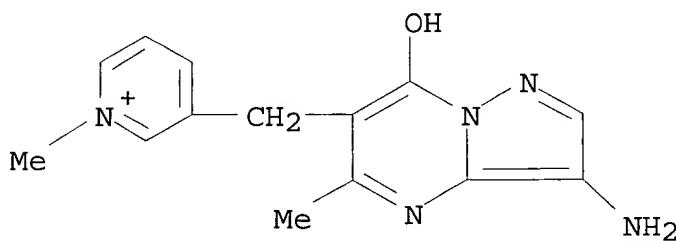
RN 286373-94-2 ZCAPLUS

CN Pyridinium, 3-[(3-amino-7-hydroxy-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)methyl]-1-methyl-, methyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 286373-93-1

CMF C14 H16 N5 O



CM 2

CRN 21228-90-0

CMF C H3 O4 S

Me—O—SO₃⁻

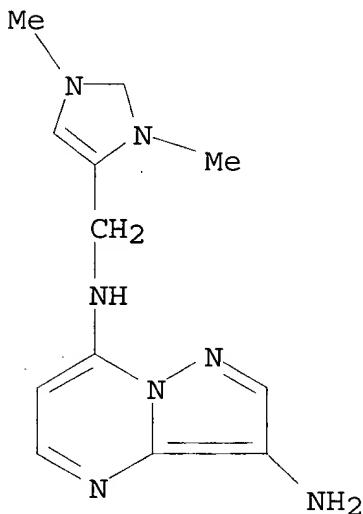
RN 286373-96-4 ZCPLUS

CN 1H-Imidazolium, 4-[(3-aminopyrazolo[1,5-a]pyrimidin-7-yl)amino]methyl]-1,3-dimethyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286373-95-3

CMF C12 H16 N7



*** FRAGMENT DIAGRAM IS INCOMPLETE ***

CM 2

CRN 21228-90-0

CMF C H3 O4 S

Me—O—SO₃⁻

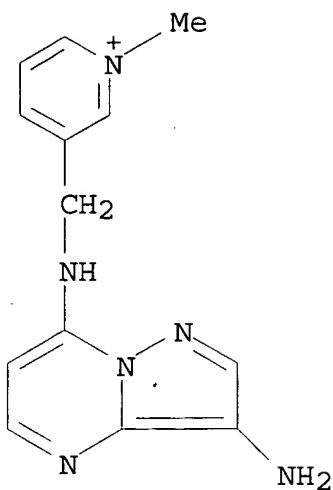
RN 286373-98-6 ZCPLUS

CN Pyridinium, 3-[(3-aminopyrazolo[1,5-a]pyrimidin-7-yl)amino]methyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286373-97-5

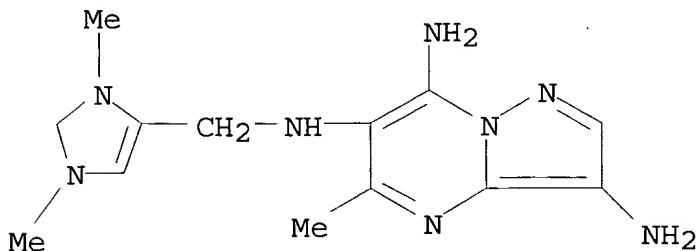
CMF C13 H15 N6



CM 2

CRN 21228-90-0
CMF C H3 O4 SMe-O-SO₃⁻RN 286374-00-3 ZCPLUS
CN 1H-Imidazolium, 4-[(3,7-diamino-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)amino]methyl-1,3-dimethyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286373-99-7
CMF C13 H19 N8

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

CM 2

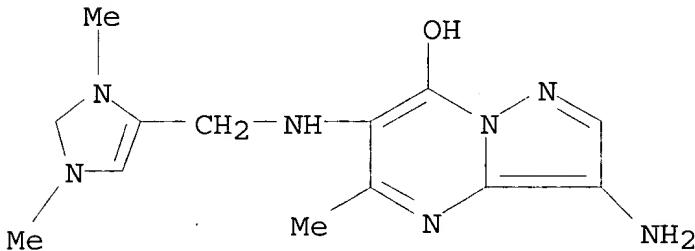
CRN 21228-90-0
 CMF C H3 O4 S

Me—O—SO₃⁻

RN 286374-02-5 ZCPLUS
 CN 1H-Imidazolium, 4-[[3-amino-7-hydroxy-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)amino]methyl]-1,3-dimethyl-, methyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 286374-01-4
 CMF C13 H18 N7 O



*** FRAGMENT DIAGRAM IS INCOMPLETE ***

CM 2

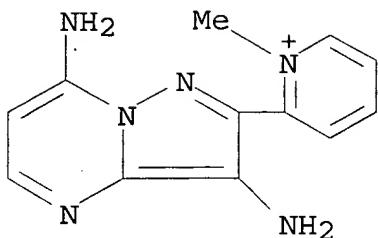
CRN 21228-90-0
 CMF C H3 O4 S

Me—O—SO₃⁻

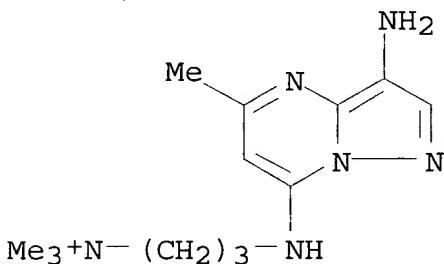
RN 286374-04-7 ZCPLUS
 CN Pyridinium, 2-(3,7-diaminopyrazolo[1,5-a]pyrimidin-2-yl)-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286374-03-6
 CMF C12 H13 N6

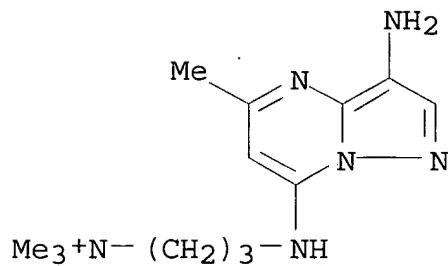


CM 2

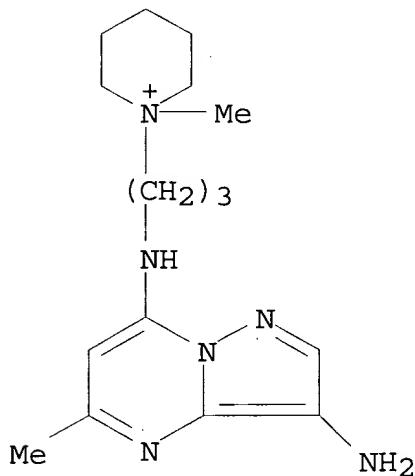
CRN 21228-90-0
CMF C H3 O4 SMe—O—SO₃⁻RN 286374-05-8 ZCPLUS
CN 1-Propanaminium, 3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)● Cl⁻RN 286374-07-0 ZCPLUS
CN 1-Propanaminium, 3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]-N,N,N-trimethyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

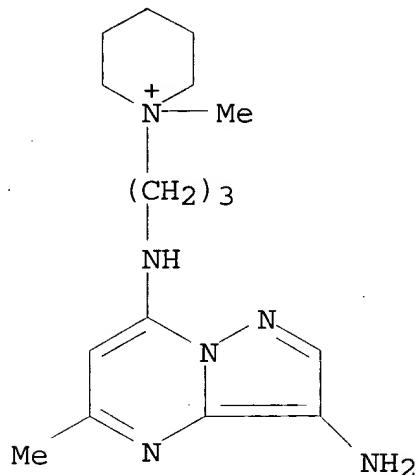
CRN 286374-06-9
CMF C13 H23 N6



CM 2

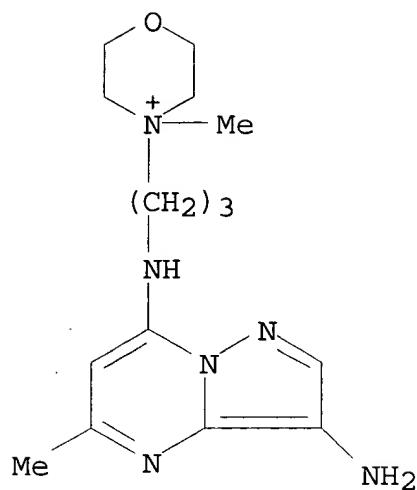
CRN 21228-90-0
CMF C H₃ O₄ SMe—O—SO₃⁻RN 286374-08-1 ZCPLUS
CN Piperidinium, 1-[3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)RN 286374-10-5 ZCPLUS
CN Piperidinium, 1-[3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286374-09-2
CMF C16 H27 N6

CM 2

CRN 21228-90-0
CMF C H3 O4 SMe-O-SO₃⁻RN 286374-11-6 ZCPLUS
CN Morpholinium, 4-[3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-4-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

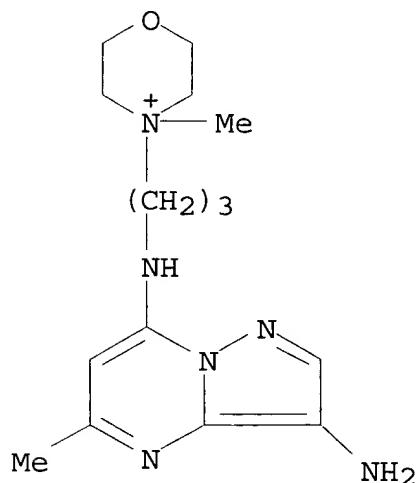
RN 286374-13-8 ZCPLUS

CN Morpholinium, 4-[3-[(3-amino-5-methylpyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-4-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 286374-12-7

CMF C15 H25 N6 O

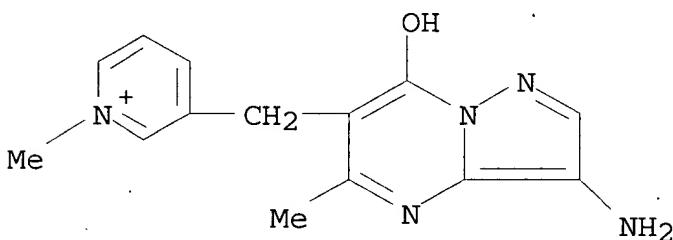


CM 2

CRN 21228-90-0
 CMF C H3 O4 S

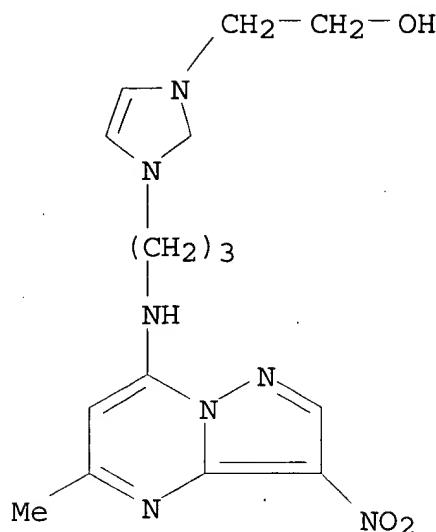
Me—O—SO₃[—]

RN 286374-14-9 ZCPLUS
 CN Pyridinium, 3-[(3-amino-7-hydroxy-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl[—]

IT 286373-86-2P
 (quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)
 RN 286373-86-2 ZCPLUS
 CN 1H-Imidazolium, 1-(2-hydroxyethyl)-3-[3-[(5-methyl-3-nitropyrazolo[1,5-a]pyrimidin-7-yl)amino]propyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

IT 286373-91-9P

(quaternary ammonium base precursor; quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)

IT 286373-84-0P 286373-87-3P 286373-92-0P
 286373-94-2P 286373-96-4P 286373-98-6P
 286374-00-3P 286374-02-5P 286374-04-7P
 286374-05-8P 286374-07-0P 286374-08-1P
 286374-10-5P 286374-11-6P 286374-13-8P
 286374-14-9P

(quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)

IT 286373-86-2P

(quaternary ammonium oxidn. bases with a pyrazolo[1,5-a]pyrimidine structure as precursors for oxidn. dyeing of hair)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT.